CLAIMS

1. A method for predicting pharmacokinetic properties of molecules comprising the steps of:

(a) preparing 2D-structures of molecules used as a training set;

(b) constructing a 2D-fingerprint by counting the number of structural descriptors that potentially relate to a pharmacokinetic property, either manually or automatically using internally developed macro; wherein said structural descriptors consist of predefined 20 to 80 atoms/fragments or substructures;

(c) analyzing the obtained 2D-fingerprint by a statistical analysis method to correlate with the pharmacokinetic property of the molecule to yield a quantitative structure-property relationship (QSPR) model; and

(d) calculating the pharmacokinetic property of a trial molecule using the above obtained QSPR model.

2. A method of Claim 1, wherein the pharmacokinetic property is absorption.

3. A method of Claim 1, wherein the pharmacokinetic property is distribution.

4. A method of Claim 1, wherein the pharmacokinetic property is metabolism

5. A method of Claim 1, wherein the pharmacokinetic property is excretion.

6. A method of Claim 1, wherein the internally developed macro comprises the macro script 2dfp.spl or 2dfp_abs.spl, written in SYBYL™ Programming Language (SPL).

7. A system for predicting pharmacokinetic properties of molecules comprising:

(a) means for preparing 2D-structures of molecules used as a training set;

(b) means for constructing a 2D-fingerprint by counting the number of structural descriptors that potentially relate to a pharmacokinetic property, wherein said structural descriptors consist of predefined 20 to 80 atoms/fragments or substructures;

(c) means for analyzing the obtained 2D-fingerprint by a statistical analysis method to correlate with the pharmacokinetic property of the molecule to yield a quantitative structure-property relationship (QSPR) model; and

(d) means for calculating the pharmacokinetic property of a trial molecule using the above obtained QSPR model.